4-Hydroxybenzoic acid 99-96-7 | DTXSID3026647

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 7.78

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.31e-01

Nearest Neighbors from the Training Set

Image not found

4-Hydroxybenzoic acid

Measured: 8.08 Predicted: 7.78

Image not found

Salicylic acid

Measured: 7.44 Predicted: 7.60

Image not found

Methylparaben

Measured: 8.57 Predicted: 7.06

Image not found

1-Octanol

Measured: 6.03 Predicted: 5.95 Image not found

Cyclohexanol
Measured: 5.18
Predicted: 4.72